ISSN NO. 2320-5407

Journal homepage: http://www.journalijar.com

INTERNATIONAL JOURNAL OF ADVANCED RESEARCH

RESEARCH ARTICLE

Band Structure and Density of States Computational Analysis of mSWCNT for different Structural Parameters

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Manuscript Info

Manuscript History:

Received: 14 May 2015
Final Accepted: 29 June 2015
Published Online: July 2015

Key words:

Breeding mSWCNT, Zigzag nanotube, nearest neighbor tight binding approximation, Linear combination of atomic orbitals, Density of states, Band structure.

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Abstract

The paper intends to present band structure, density of states and lowest subband P_z tight binding computational analysis of mSWCNT. As the criterion is limited to metallic SWCNT hence armchair chirality is considered and analytical computation utilizes nearest neighbor tight binding (NNTB) approximation. The parameters of DOS are obtained by varying cylindrical dimension. The results conclude the dependence of peak of DOS on CNT's physical dimensions such as tube radius, bandgap reduction and decrement of nearest neighbor distance.

INTRODUCTION

The sub100 nm regime subjects increasing challenges for both active and passive components on the chip. The continuous scaling of the feature sizes of transistors and interconnects, increase in transistor speed, propagation delays, increment in contact resistance etc. have become the dominant chip performance limiting factor [1]. Consequently, materials such as carbon nanotubes (CNTs), graphene, nanoribbons, and Ag nanowires are being considered as potential replacements for Cu in interconnects, due to their better electrical and mechanical properties [1]. CNT appears to be the most promising to replace Cu due to its ultrahigh current capacity and it's filling ability in high aspect ratio structures. mCNTs are verified to possess high current carrying ability and conductance approaches the theoretical limit at small biases. Their low resistance and strong mechanical properties make them viable as interconnects in both silicon nanoelectronics and molecular electronics as depicted in fig.1.

The invention of CNT [6], introduced a great leap in the electronics industry as it provided a constructive approach to meet the ever-increasing demand of high frequency and high level integration of electronic devices and circuits. Specific to interconnections the shift to nanometer regime aggravates the problem as in deep submicron regime more number of interconnections are used to connect millions of devices increasing wire resistance and giving rise to propagation delay. Earlier Al & Cu interconnects were viable enough, but the shrinking of device dimensions caused these conventional interconnects to suffer from problems like high electromigration resistance, surface roughness, grain boundary scattering, interconnect scaling, multiple interconnect stacks, leakage power, support to FinFET etc.

Carbon nanotubes (CNTs) offer an attractive option for VLSI interconnect applications as they have remarkable electrical, mechanical, thermal properties and large current-carrying capability due to their small dimensions [7]–

[11]. This novel interconnect technology has the potential to replace copper in future. However, there occurs some significant technical barriers for using CNTs as building blocks in nanoelectronics [12]. Hence, a pragmatic analysis of the same becomes essential to evaluate their performance in the domain of on-chip interconnections.

Apart from being metallic in nature their high thermal and mechanical stability, thermal conductivity of around 5800W/mK and current density of 1014A/m2 even at temperatures higher than 200 ℃ and Fermi velocity comparable with that of a metal suggest them to be a good supplement as VLSI interconnects. However, as we approach the nanometer regime conventional interconnects such as Cu and Al are exposed to problems like electronmigration subjected to breakdown when current densities exceed 106 A/cm2. Nanotube arrays on the other hand can be integrated with silicon technology and holds great possibilities as vertical vias (3D interconnects) carrying current more than an order of magnitude larger current densities than conventional vias [21, 22]. Studies reveal that mSWCNT with diameters as small as 5 Å propose as good interconnects and nanoscale contacts from the perspective of molecular electronics [23].

It has been realized that band structure and density of states of a quantum structure convincingly describe the electrical characteristics of nanostructure based devices which results in accurate device designs [5].

Amongst MWCNT, DWCNT and SWCNT, mSWCNT in isolated and bundled form are preferred for interconnect applications owing to their simple fabrication and enhanced stability [13]. Armchair configuration of SWCNT is the preferred option for interconnect application owing to its metallic nature hence the paper intends to analyze the same.

CNT cylindrical growth results from monoatomic layer of graphene with diameter of nanometer range. The tubes are of metallic or semiconductor behavior depends on their chirality. SWCNTs of armchair configuration are metallic in nature where the two integer n and m are equal. In terms of n and m, the magnitude of chiral vector is [3]:

$$\overrightarrow{C_h} = a\sqrt{n^2 + m^2 + nm} \quad (1)$$

which is also the measure of its circumference.

DOS profile of CNT includes a set of peaks symmetrical w.r.t Fermi level [14] where DOS and band structure depends on wave-vector [15-18], which provides the dependency of DOS and band structure on wave-vector. Consequently, the paper intends to present band structure and density of states computational analysis of mSWCNT. As the criterion is limited to metallic SWCNT hence armchair chirality is considered and analytical computation utilizes nearest neighbor tight binding (NNTB) approximation and theory of linear combination of atomic orbitals (LCAO) where the parameters of DOS are obtained by varying cylindrical dimension. The results conclude the dependence of DOS peak limits on CNT's physical dimensions such as tube radius, bandgap and nearest neighbor distance.

Mathematical modelling for mSWCNT

1. The diameter (d) of the SWCNT bundled interconnect are selected such that they are confined within the range from 0.7 to 5 nm i.e. for SWCNT and $d \leq 2.5$ nm to exclude any possibility of including MWCNT [19]. Their values are 2.1696nm, 2.3042nm and 2.4408nm.
2. The above mentioned values of diameter are specifically selected based on their chirality's 16,17 and 18 respectively and tube diameters are realized using expression:

   Diameter of Tube $= \frac{\gamma}{\pi} = \sqrt{n^2 + nm + m^2}$ (2)

   where $\gamma = \sqrt{3}a_{cc}$ where $a_{cc} = 0.142nm$
3. The results obtained using CNT bands are tabulated in table 1.1 and are utilized to obtain the results for the below mentioned sections.

Band structure of mSWCNT

SWCNTs are one-dimensional (1D) and exhibit unique electrical and transport properties owing to their electronic band structures, small size and low dimension. SWCNT is defined by the coordinates of its chiral (wrapping) vector denoted by indices n and m which dictates the extent of lattice vectors al and a2 of the graphene lattice required for a specific chiral vector. The nanotube's diameter indicates the length of chiral vector divided by n while the chiral angle is the measure between the chiral vector and basis vector al. The range of chiral angle is between 0° for zigzag structure to 30°for armchair structures [10].

mSWNTS are metallic in nature as their n-m value is equal to zero which can be easily verified by the present model which considers the three n, m values such as 16, 17 and 18 resulting in diameters of 2.1696nm, 2.3042nm and 2.4408nm respectively. The band structure with respect to the mentioned dimensions are illustrated in fig.2.

The above illustration in fig.2 explains the bandstructure and transmission versus the electron energy of a single wall armchair metallic nanotube. Various subbands arising from quantization of the wave vector around the circumference of the nanotube are indicated where the transmission changes by an integer when a subband opens or closes. It is quite vivid that the magnitude of transmission change corresponds to the subband degeneracy. It also indicates that the number of subbands increases with an increase in the nanotube diameter owing to an increment in the total number of quantum numbers arising from quantization of the electron wave function around the nanotube circumference. [20]

As there is a minor symmetry between the conductance and valence bands, the Fermi energy is at the zero of energy in fig.2 where the subbands cross and is independent of nanotube diameter. The location of the wave vector (k), where this crossing point occurs changes with nanotube chirality and the subbands are known as crossing subbands as mentioned in fig.2.There exists only two subbands per spin at the Fermi energy which are independent of nanotube diameter and chirality. It is also viewed that the energy of the first semiconducting subbands from the Fermi energy decreases inversely with the increase in nanotube diameter. [20]

Density of States of mSWNTs

DOS estimates the optical properties of carbon nanotubes obtained from electronic transitions within 1D density of states (DOS). It is not a continuous function of energy, rather descends gradually and then increases in a discontinuous spike with sharp peaks known as Van Hove singularities. The energies between the Van Hove singularities depend on the nanotube structure which can be varied to tune the optoelectronic properties of carbon nanotube.

The density of states can be expressed as:

$$D(E) = \frac{\sqrt{3}a^2}{2\pi R}\sum_i \int dk\delta(k - k_i)\left|\frac{\partial\varepsilon}{\partial k}\right|^{-1} \text{ where } \varepsilon(k_i) = E. \quad (3)$$

The results presented in Fig. 3 shows the DOS calculated with respect to variation in diameters of mSWCNT based on chirality i.e. (16,16),(17,17) and (18,18) realizing the presence of singularities at the band edges.

The expansion of dispersion relation around the Fermi point results (4) [24]

$$D(E) = \frac{a\sqrt{3}}{\pi^2 R\gamma}\sum_{m=1}^{N}\frac{|E|}{\sqrt{E^2-\epsilon_m^2}} \text{ where, } \varepsilon_m = |3m|(a\gamma/2R) \text{ for metallic tubes} \quad (4)$$

The above mentioned expression (4) for the density of states expresses van Hove singularities when E = ±εm, indicative of quasi-one-dimensional materials (fig.3). The presence of these singularities in DOS are authenticated by STM of individual nanotubes [25].

Lowest subband Pz tight binding in mSWCNT

A tight binding model includes one p_Z orbital per carbon atom and the nearest neighbour interaction is utilised to calculate the graphene band structure. An extensive calculations that includes multiple orbitals and more levels of neighbouring atoms expresses one-orbital, tight-binding approximation compatibility at the energy range near the Fermi point of the graphene sheet, the region of interest for electronic transport [16].The E-k relation describes the eigen-energies of the plane wave state in a periodic crystal lattice which necessitate the expression of the wave vector-dependent Hamiltonian for one unit cell, treating the C-C bonding within the unit cell itself and the bonding with neighbouring unit cells.

The band structure of an armchair tube in the tight binding p_z orbital is expressed utilizing the expression:

$$E = \pm t_0\sqrt{1 + 4cos\left(\frac{v\pi}{n}\right)cos\left(\frac{k\sqrt{3}a_{cc}}{2}\right) + 4cos^2\left(\frac{k\sqrt{3}a_{cc}}{2}\right)} \quad (5)$$

where, t_0 = 2.6eV is the hopping parameter, acc = 1.42 × 10^{-10}m is the c-c bonding distance, and the (+) and (−) signs symbolizes the conduction and valence bands respectively. At, υ= 0 the conduction and valence bands cross each other near the Fermi points:

$$k_f = \pm\frac{2\pi}{3\sqrt{3}a_{cc}} \text{ expressing the metallic nature to the armchair tube} \quad (6)$$

On substituting υ=0, $k = k_t + 3k_0/2$ in Eq. 5, we get:

$$E = \pm t_0 \left(1 - 2cos\left(\frac{k_t\sqrt{3}a_{cc}}{2}\right)\right) \text{ where, } k_0 = 2k_F = \frac{4\pi}{\sqrt{3}a_{cc}} \approx 1.7 \times 10^{10}/\text{m} \quad (7)$$

The expression (7) resulting in the value of 2.598 eV which can also be verified from fig.4.

The metallic bands based on above expressions are depicted in Fig.4 shows these metallic bands, the k− space, and the Brillouine zone of armchair tube. At the Γ point, conduction band energy is $E_c = -t_0 = -3$eV and the crossing of the conduction and valence bands occur at $k_t = \pm 0.66k_0$ also mentioned in table1.

Results and Discussion

The results obtained and presented expresses the band structure, density of states and metallic band representation of armchair single-wall carbon nanotube. The results obtained analytically as function of nearest neighbor distance and radius of the cylindrical structure expresses the effect of geometrical specifications on electrical performance. Hence a proper choice of design parameters can be made from the available results to design armchair SWCNT-based electronic or optoelectronic devices.

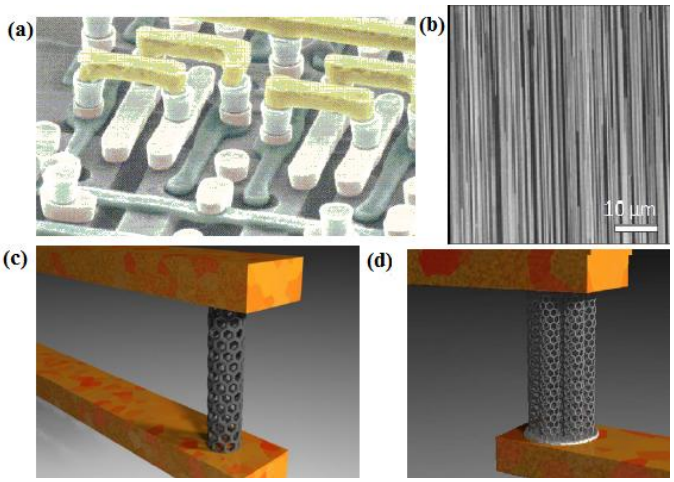

Fig.1 (a) Illustration of the wiring in an integrated circuit depicting horizontal interconnects (yellow) and vertical interconnects (grey). (b) An example of a SWNT array , which can potentially be used as a vertical interconnect provided excellent electrical contacts can be made to both the top and bottom of the nanotube array. (c) Illustration of the limit where a SWNT is used as a vertical interconnect in what may eventually become a molecular circuit. (d) Bundled SWCNT based interconnect will have a low bias resistance of 6.5 k divided by the number of nanotubes. (Source: (a) IBM Journal of Research and Development, (b) Kocabas Research Group Laboratory of Quantum Electronics, (c) and (d) courtesy of Infineon Technologies.)

Table1: Chirality dependent input/output parameters of mSWCNT

	Parameters	Chirality(m,n)		
		(16,16)	(17,17)	(18,18)
I.	Basic Input Parameters			
1	Carbon center to center distance (Å)	1.42	1.42	1.42
2	Tight binding overlap integral (eV)	3	3	3
II.	Basic Output Parameters			
1.	Nanotube diameter (nm)	2.1696	2.3052	2.4408
2.	Nanotube circumference (nm)	27.713	29.445	31.177

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3.	Chiral angle (degrees)	30	30	30
4.	Length of unit cell (nm)	0.24595	0.24595	0.24595
5.	Number of hexagons (unit cell)	32	34	36
6.	Boundary of Brillouin Zone (k_{tmax})	1.28E+10	1.28E+10	1.28E+10
7.	Bandgap Magnitude (eV)	0.01088	0.01088	0.01088
8.	Bandgap Magnitude in units of overlap parameter (t)	0.0036265	0.0036265	0.0036265
9.	k_t at bandgap	-0.666	-0.666	0.666

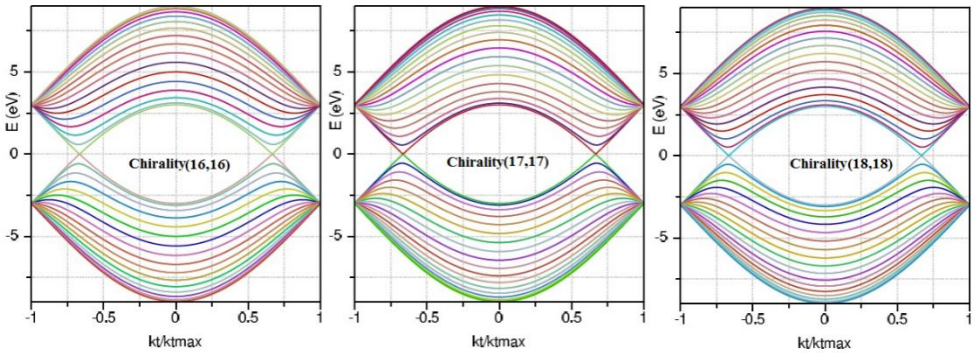

Fig.2: Band structures of metallic single walled carbon nanotubes.

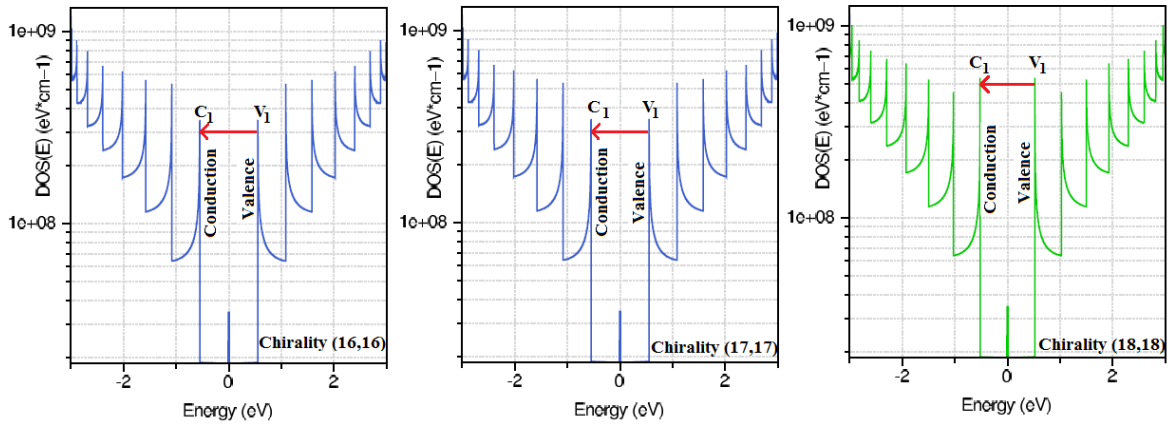

Fig. 3 Density of states for (16, 16), (17, 17) and (18, 18) CNTs computed from tight binding showing van Hove singularities.

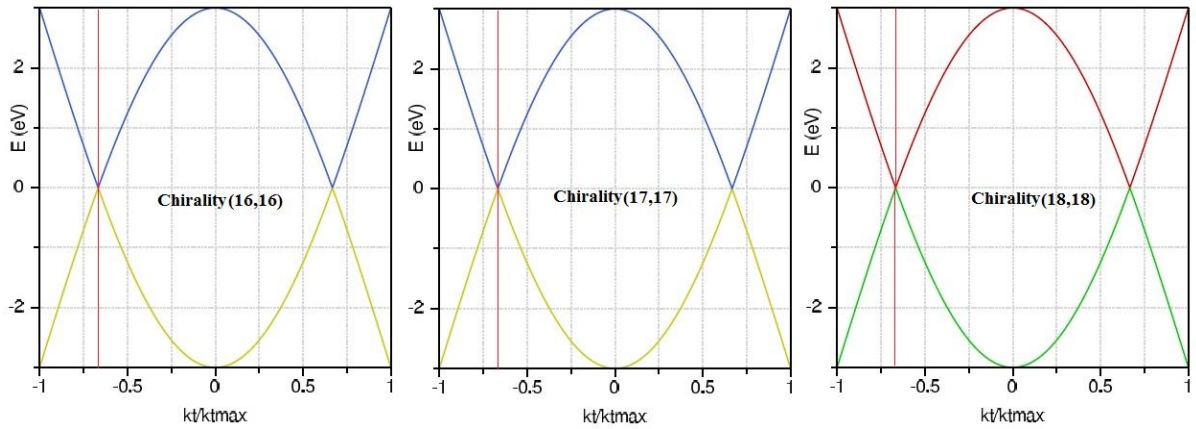

Fig.4: Metallic band E-k/ktmax in armchair tubes with chiral vectors (16, 16), (17, 17) and (18, 18)

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